Nanohydrodynamics Simulations: An Atomistic View of the Raleigh-Taylor Instability

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The Rayleigh-Taylor (RT) instability occurs when a heavy fluid lies on top of a light fluid in the attendance of a gravitational field g; the fluids will subsequently mix in a more or less turbulent process. The RT process is the classical example of turbulence and was first investigated by Lord Rayleigh in 1883 and later, theoretically, by Taylor. Its relevance ranges from astrophysical supernova explosions, to geophysical formations like salt domes and volcanic islands, all the way down to inertial confinement fusion, as well as to the general turbulent mixing of fluids.

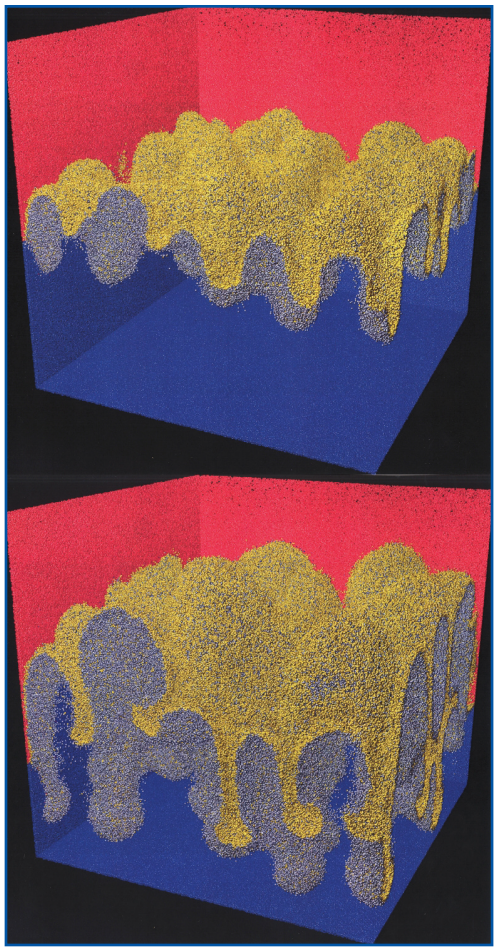

Figure 1—
Rayleigh-Taylor mixing of 100,589,840 atoms by molecular dynamics of a heavy fluid (red/yellow spheres) on top and a light fluid (blue/gray spheres) below, under the influence of a gravitational field. The predicted most unstable mode emerges quickly for an interface initially perturbed only by thermal fluctuations (upper panel, time = 18t0). Spikes and bubbles grow mushroom caps and start to interact with each other (lower panel, time = 24t0). Only atoms at the interface of the two fluids are shown (yellow/gray), red and blue atoms mark the boundaries of the simulation box.

Molecular dynamics simulations have been performed on the well-studied RT instability as an example and validation of nanohydrodynamics [1]. Raleigh-Taylor simulations require a large number of particles in an MD calculation to resolve fluid structures at late times, as well as the imposition of an enormous gravitational field, in order to reduce the most unstable wavelength to the nanoscale, as well as to mix the fluids on the nanosecond time scale. This most unstable mode of wavelength l must be several times smaller than the width of the simulation cell in order to develop several bubbles and spikes. From linear stability analysis, the most unstable wavelength decreases with increasing g, and thus a value of g approximately 10 billion times larger than the gravity on Earth is required. Whether such a large g distorts the instability process depends on whether g is a scalable variable up to that magnitude, which can be validated by comparison to experiment and to continuum descriptions of the hydrodynamical problem as described by the Navier-Stokes (NS) equations, which assume scalability.

Using 1600 CPUs of the Advanced Simulation and Computing (ASC) Q computer system at Los Alamos National Laboratory (LANL), we simulated 100,589,840 atoms (Fig. 1) for 250,000 integration time steps (400,000 CPU hours) with the Scalable Parallel Short-range MD (SPaSM [2]) code. Smaller simulations were performed on the ASC QSC computer system (1024 CPUs), and a 256-CPU Linux cluster (Grendels) at LANL. The simulations presented here needed an estimated total of 600,000 CPU hours. Accounting for different processor speed on the used systems this is more than a week on all 4096 CPUs of the ASC Q computer system.

The growth from an interface perturbed only by fluctuations was found to be dominated quickly by the wave number corresponding

to linear stability analysis, which then determines the initial number of bubbles and spikes (Fig. 1). For example, the fully 3D system should, according to linear stability analysis, have 3.5 spikes along the edge of the simulation cell, while actually 4 were observed at early times. In some cases the deviations from the theoretically most unstable mode predictions were larger due to the presence of multiple modes and the finite edge length. At later times the spikes and bubbles develop mushrooms at their tips, which eventually interact and merge in a process that can be described as turbulent (see movie on the Web [1]). The penetration distance h of the spikes and bubbles is characterized at long times by the coefficient alpha (Fig. 2). Somewhat surprisingly, there was no statistically significant difference between the average value of alpha, as determined from the large number of simulations done with a slab geometry at Atwood Number A = 0.867 and a single fully 3D system. The growth of the bubbles and spikes as given by the value of alpha determined by the simulations were found to agree with experiment as well as Youngs' theoretical model (Fig. 3). This remarkable quantitative agreement with experiment at late times (in the turbulent regime) is a significant validation of nanohydrodynamics. At the longest time of penetration of the spikes in the simulations, the depth reached 30% of the experimental value, measured in terms of the most unstable wavelength. Different continuum hydrodynamic calculations show a range of alpha values for bubbles between 0.03 and 0.08, compared to an experimental range of 0.05 to 0.08.

With MD simulation it is possible to quantitatively determine how alpha depends on initial conditions, such as the surface tension and imposed disturbances. It was found that the alpha values of the spikes in the miscible case are reduced compared to the immiscible case at high Atwood number. In the miscible case, the interface gets blurred by diffusion. This can be interpreted as a reduction of the effective Atwood number, leading to a reduction in the alpha of the spikes but not bubbles, since their alpha value

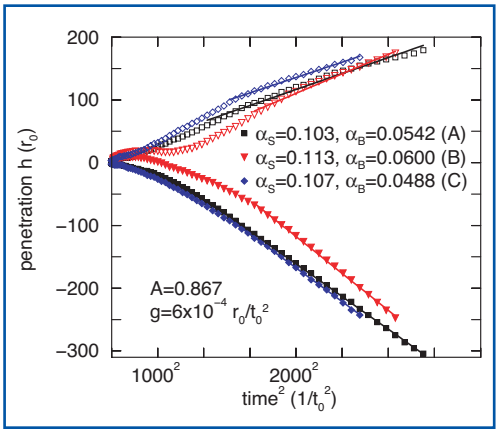

Figure 2—
Penetration h of bubbles (open symbols) into the heavy fluid and spikes (closed symbols) into the light fluid as a function of the square of the time at Atwood number. The long-time slope of the growth rate alpha (solid lines) of the thin slab (A: black squares) and the fully 3D MD simulation (B: red triangles) are, to within statistical error, the same. An initial single mode perturbation with wavelength l = 70r0 and amplitude d = 0.02l (C: blue diamonds) does not change the long-term slope. However, when l is not small compared to the system height H = 612.5r0 (and thus the fall height of spikes and bubbles) the mixing can be enhanced (not shown).

is nearly independent of A. It was also found that an initial single-mode perturbation of the interface enhances the mixing process at short times—an effect also observed experimentally. However, at distances large compared to the initial perturbing mode, the effect is washed out, and alpha is similar to the value from a fluctuation-perturbed interface. This suggests a memory loss about the initial perturbations in time in the atomistic simulations due to the chaotic nature of the underlying equations of motions.

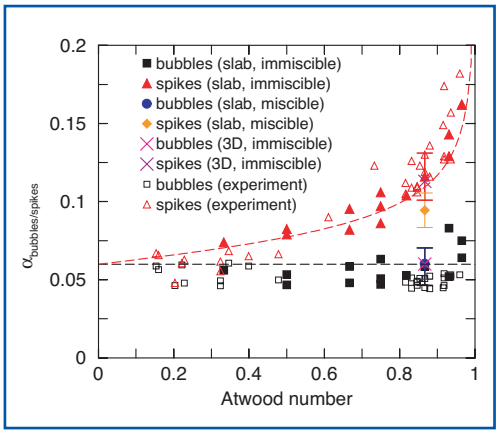

Figure 3—
The alpha values for various Atwood numbers A from MD simulations compared to experimental data [3], and Youngs' model with C = 3.67 (dashed lines). For large A, alpha approaches the free fall value of 0.5 at A = 1. At A = 0.867, 3 miscible and 19 immiscible simulations were made and the error bars indicate the standard deviation, rather than the smaller confidence interval.

[1] K. Kadau, T.C. Germann, P.S. Lomdahl, B.L. Holian, Guy Dimonte, Nicolas G. Hadjiconstantinou, and Berni Alder, *PNAS* **101**, 5851 (2004).
[2] P.S. Lomdahl, P. Tamayo, N. Gronbech-Jensen, and D.M. Beazley, *Proceedings of Supercomputing* **93**, G.S. Ansell, Ed. (IEEE Computer Society Press, Los Alamitos, CA, 1993), p. 520.
[3] G. Dimonte and M. Schneider, *Phys. Fluids* **12**, 304 (2000).